D_{4h}^{18} $I4/m2/c2/m$ No. 140 $I4/mcm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
32 *m* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
	(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
	(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
	(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2m$ (121)	(1; 2; 5; 6; 11; 12; 15; 16)+		$0,1/2,1/4$
[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+		
[2] $I4cm$ (108)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[2] $I422$ (97)	(1; 2; 3; 4; 5; 6; 7; 8)+		$0,0,1/4$
[2] $I4/m11$ (87, $I4/m$)	(1; 2; 3; 4; 9; 10; 11; 12)+		
[2] $I2/m2/c1$ (72, $Ibam$)	(1; 2; 5; 6; 9; 10; 13; 14)+		
[2] $I2/m12/m$ (69, $Fmmm$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_2/ncm$ (138)	1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,3/4,1/4$
[2] $P4_2/mbc$ (135)	1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,0$
[2] $P4_2/nbc$ (133)	1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,3/4,1/4$
[2] $P4_2/mcm$ (132)	1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,0$
[2] $P4/ncc$ (130)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,1/4$
[2] $P4/mbm$ (127)	1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P4/nbm$ (125)	1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,1/4$
[2] $P4/mcc$ (124)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16		

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I4/mcm$ (140)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I4/mcm$ (140)	$\langle 2;\ 3;\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I4/mcm$ (140)	$\langle 2;\ 3;\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$

$I4/mcm$ (140)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 9+(0,0,2u)\rangle$ prime $p>2$; $0\le u<p$ p conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$

$I4/mcm$ (140)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ prime $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Fm\bar{3}c$ (226)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4/mmm$ (123, $P4/mmm$)

